# Sebacic acid, isobutyl 4-(2-phenylpropyl-2)-phenyl ester

**Inchi:** InChI=1S/C29H40O4/c1-23(2)22-32-27(30)16-12-7-5-6-8-13-17-28(31)33-26-20-18-25(1

**InchiKey:** IUUPLMXJADRNIM-UHFFFAOYSA-N

**Formula:** C29H40O4

**SMILES:** CC(C)COC(=O)CCCCCCCCC(=O)Oc1ccc(C(C)(C)c2ccccc2)cc1

**Mol. weight [g/mol]:** 452.63

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -58.95 | kJ/mol | Joback Method |
| hf | -683.93 | kJ/mol | Joback Method |
| hfus | 53.20 | kJ/mol | Joback Method |
| hvap | 101.99 | kJ/mol | Joback Method |
| log10ws | -8.04 | | Crippen Method |
| logp | 7.238 | | Crippen Method |
| mcvol | 386.830 | ml/mol | McGowan Method |
| pc | 954.96 | kPa | Joback Method |
| rinpol | 3503.00 | | NIST Webbook |
| rinpol | 3503.00 | | NIST Webbook |
| tb | 1070.17 | K | Joback Method |
| tc | 1310.26 | K | Joback Method |
| tf | 613.69 | K | Joback Method |
| vc | 1.474 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1322.95 | J/mol×K | 1070.17 | Joback Method |
| cpg | 1338.17 | J/mol×K | 1110.18 | Joback Method |
| cpg | 1351.93 | J/mol×K | 1150.20 | Joback Method |
| cpg | 1364.36 | J/mol×K | 1190.21 | Joback Method |
| cpg | 1375.57 | J/mol×K | 1230.23 | Joback Method |
| cpg | 1385.68 | J/mol×K | 1270.24 | Joback Method |
| cpg | 1394.80 | J/mol×K | 1310.26 | Joback Method |
| dvisc | 0.0001701 | Pa×s | 613.69 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000818 | Pa×s | 689.77 | Joback Method |
| dvisc | 0.0000455 | Pa×s | 765.85 | Joback Method |
| dvisc | 0.0000282 | Pa×s | 841.93 | Joback Method |
| dvisc | 0.0000189 | Pa×s | 918.01 | Joback Method |
| dvisc | 0.0000134 | Pa×s | 994.09 | Joback Method |
| dvisc | 0.0000100 | Pa×s | 1070.17 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U354544&Units=SI |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |